Mechanical Engineering Doctoral Defense

Study of interface adhesive properties of wurtzite materials for carbon fiber composites

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abstract

Recently, the use of zinc oxide (ZnO) nanowires as an interphase in composite materials has been demonstrated to increase the interfacial shear strength between carbon fiber and an epoxy matrix. In this research work, the strong adhesion between ZnO and carbon fiber is investigated to elucidate the interactions at the interface that result in high interfacial strength. First, molecular dynamics (MD) simulations are performed to calculate the adhesive energy between bare carbon and ZnO. Since the carbon fiber surface has oxygen functional groups, these were modeled and MD simulations showed the preference of ketones to strongly interact with ZnO, however, this was not observed in the case of hydroxyls and carboxylic acid. It was also found that the ketone molecules ability to change orientation facilitated the interactions with the ZnO surface. Experimentally, the atomic force microscope (AFM) was used to measure the adhesive energy between ZnO and carbon through a liftoff test by employing a highly oriented pyrolytic graphite (HOPG) substrate and a ZnO covered AFM tip. Oxygen functionalization of the HOPG surface is shown the increase of adhesive energy. Additionally, the surface of ZnO was modified to hold a negative charge, which demonstrated an increase in the adhesive energy. This increase in adhesion resulted from increased induction forces given the relatively high polarizability of HOPG and the preservation of the charge on ZnO surface. It was found that the additional negative charge can be preserved on the ZnO surface because there is an energy barrier since carbon and ZnO form a Schottky contact. Other materials with the same ionic properties of ZnO but with higher polarizability also demonstrated good adhesion to carbon. This result substantiates that their induced interaction can be facilitated not only by the polarizability of carbon but by any of the materials at the interface. The versatility to modify the magnitude of the induced interaction between carbon and an ionic material provides a new route to create interfaces with controlled interfacial strength.

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